

**Berciu and Bhatt reply:** The point raised by the authors of the Comment [1] regarding the hopping term  $t(r)$  we use [2] to describe the impurity band (IB) of holes in  $\text{Ga}_{1-x}\text{Mn}_x\text{As}$ , needs clarification. A proper description of the hopping between impurity states in such alloys is a very complicated and, to our knowledge, unsettled issue. In our work, we used a hopping parameter of magnitude corresponding to two isolated s-wave impurities, with  $t(r) < 0$  in the hole representation. This parametrization captures two important length scales - the inter Mn-Mn distance, and the impurity Bohr radius - present in a complete model of the experimental system. With our parameters, in the absence of magnetization, we obtain an impurity band for holes whose density of states (DOS) is plotted in Fig.1 (left), for a Mn concentration  $x = 0.93\%$  using the impurity Rydberg (Ry) as a unit ( $1\text{Ry}=112\text{ meV}$  for Mn in GaAs). The top of the hole impurity band is 3 Ry above the valence band, while the Fermi energy  $E_F$  for holes lies 2.5 Ry above the top of the valence band. These appear to be reasonable numbers: for a random distribution of acceptor centers A, the top of the hole band would be expected to correspond to the ionization potential of the most stable configuration, which is likely an  $A_4$  complex accomodating 4 holes in the ground impurity state. In a hydrogenic model, this is  $\approx 4.5\text{ Ry}$  [3]; for centers with strong central cell like Mn in GaAs, it is likely reduced somewhat. In the mean-field approach, this is the situation above  $T_c$ , while for  $T < T_c$ , the coupling to the Mn spins causes the spin up and down bands to split, leaving the system fully polarized at  $T = 0$  (see inset).

Additionally, with the parameters used the IB shows a mobility edge close to  $E_F$ , as demonstrated by computing the inverse participation ratio  $\text{IPR} = \sum_i |\phi(i)|^4$ , where  $\phi(i)$  is the wavefunction amplitude at site  $i$ . For an *extended* wave-function,  $\text{IPR} \sim 1/N_d$ , where  $N_d$  is the number of sites of a finite sample. For *localized* wavefunctions, the IPR is independent of system size. The average IPR for the wavefunctions of our hopping Hamiltonian are shown in Fig. 1 (right) for  $N_d = 125$  and 1000. The occupied hole states at the top of the hole impurity band are localized, with relatively high and size-independent IPR, whereas states of lower energy, which are occupied only at *higher* hole fillings, are extended with IPR's depending on size in the expected manner. Thus, the model captures the proximity of the Metal-Insulator Transition, seen in experiment. (For  $x = 5\%$ , where the magnetization is much less anomalous, the IB top is again split a few Ry above the valence band, and is somewhat wider).

On the other hand, as pointed out in the Comment [1], the choice  $t(r) > 0$  in the hole picture, which inverts the IB ( $E \rightarrow -E$ ), is not suitable because it leads to an unphysical long tail of the DOS in the gap at the densities of interest, and a consequent low DOS at  $E_F$ . Moreover, all the relevant states are extended (there is no mobility edge). A more realistic calculation of the IB, including

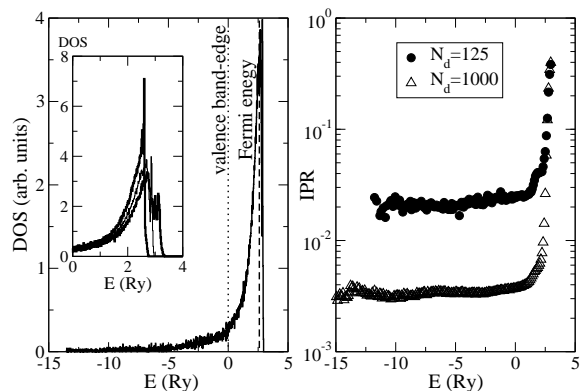


FIG. 1. Left: DOS for hopping Hamiltonian with  $t(r) < 0$ . The inset shows the effect of the AFM coupling ( $J = 15\text{ meV}$ ). The  $\sigma = \uparrow$  and  $\sigma = \downarrow$  bands (thick lines) are no longer degenerate at low temperatures. For comparison, we plot the  $J = 0$  DOS as well (thin line). Right: dependence of the average IPR on the energy. In both pictures  $x=0.0093$ .

the Coulomb potential from the other Mn impurities as well the charged impurities responsible for the large compensation, and using the more complicated structure of a *hole* impurity wavefunction, will likely remove the unphysical tail and yield a DOS similar to the one used in our calculation, with proximity to a mobility edge. Already the tail is absent in *e.g.* Ref. 3, for a hydrogenic lattice. Since the nature of compensation in GaMnAs is still an open question, we opted to use a simple model that gives a physically acceptable description of the IB.

Our goal in Ref. [2] was to use this simple IB model to point out non-trivial effects of disorder in Mn positions on the shape of the magnetization curve  $M(T)$  and the critical temperature  $T_C$ . To our knowledge, all previously published studies had neglected this aspect. Studies appearing since support our claim of increased  $T_C$  with increased Mn disorder [4]. While we agree that a better modeling of the impurity band and inclusion of the valence band and other factors such as screening (on a proper, local scale, taking into account strong charge inhomogeneities) are necessary to achieve a proper *quantitative* description especially in the metallic regime  $x > 0.03$ , we maintain that the underlying physics captured by our simple model of Ref. [2] is essentially correct.

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- [1] C. Timm, F. Schafer and F. von Oppen, previous comment.
  - [2] Mona Berciu and R. N. Bhatt, Phys. Rev. Lett. **87**, 107203 (2001).
  - [3] R. N. Bhatt and T. M. Rice, Phys. Rev. B **23**, 1920 (1981). (See Figs. 3 and 6).
  - [4] A. L. Chudnovskiy, cond-mat/0108396; A. Millis, invited talk at Spintronics2001, Washington DC, Aug. 9-11, 2001.